

N,N-Diethylaniline
91-66-7 | DTXSID8021800

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.92

Global applicability domain: Inside

Local applicability domain index: 5.21e-01

Confidence level: 4.64e-01

Nearest Neighbors from the Training Set

Image not found

Benzenamine, N-butyl-2-methoxy-

Measured: 2.85

Predicted: 1.30

Image not found

Piperidine, 1-phenyl-

Measured: 2.98

Predicted: 1.09

Image not found

1-Phenylpyrrolidine

Measured: 3.56

Predicted: 1.46